

Isonipecotic acid, N-(2,4-difluorobenzoyl)-, pentyl ester

Inchi: InChI=1S/C18H23F2NO3/c1-2-3-4-11-24-18(23)13-7-9-21(10-8-13)17(22)15-6-5-14(19)1
InchiKey: TYFWXARLNWXYPP-UHFFFAOYSA-N
Formula: C18H23F2NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1
Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	3.550		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2457.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361367&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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